# Heptyl methyl phthalate

**Other names:** 1,2-Benzenedicarboxylic acid, heptyl methyl ester
**Inchi:** InChI=1S/C16H22O4/c1-3-4-5-6-9-12-20-16(18)14-11-8-7-10-13(14)15(17)19-2/h7-8,10-
**InchiKey:** HJOXYDMLDIRNIT-UHFFFAOYSA-N
**Formula:** C16H22O4
**SMILES:** CCCCCCCOC(=O)c1ccccc1C(=O)OC
**Mol. weight [g/mol]:** 278.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -281.22 | kJ/mol | Joback Method |
| hf | -638.11 | kJ/mol | Joback Method |
| hfus | 36.42 | kJ/mol | Joback Method |
| hvap | 72.46 | kJ/mol | Joback Method |
| log10ws | -4.47 | | Crippen Method |
| logp | 3.600 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 1816.95 | kPa | Joback Method |
| rinpol | 2039.00 | | NIST Webbook |
| rinpol | 2039.00 | | NIST Webbook |
| tb | 749.72 | K | Joback Method |
| tc | 951.49 | K | Joback Method |
| tf | 453.34 | K | Joback Method |
| vc | 0.872 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 648.45 | J/mol×K | 749.72 | Joback Method |
| cpg | 663.58 | J/mol×K | 783.35 | Joback Method |
| cpg | 677.73 | J/mol×K | 816.98 | Joback Method |
| cpg | 690.92 | J/mol×K | 850.61 | Joback Method |
| cpg | 703.17 | J/mol×K | 884.24 | Joback Method |
| cpg | 714.48 | J/mol×K | 917.86 | Joback Method |
| cpg | 724.87 | J/mol×K | 951.49 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0008522 | Pa×s | 453.34 | Joback Method |
| dvisc | 0.0004919 | Pa×s | 502.74 | Joback Method |
| dvisc | 0.0003132 | Pa×s | 552.13 | Joback Method |
| dvisc | 0.0002148 | Pa×s | 601.53 | Joback Method |
| dvisc | 0.0001560 | Pa×s | 650.93 | Joback Method |
| dvisc | 0.0001185 | Pa×s | 700.32 | Joback Method |
| dvisc | 0.0000934 | Pa×s | 749.72 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373884&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |